ELECTRONIC SPECTROSCOPY OF MASS-SELECTED $C_7H_3^+$ AND C_7H_3 ISOMERS IN 6 K NEON MATRICES

JOHN P. MAIER, ARGHYA CHAKRABORTY, JAN FULARA, *Department of Chemistry, University of Basel, Basel, Switzerland.*

Three open chain isomers of $C_7H_3^+$ including a three member carbon ring in the structure were identified in a neon matrix held at 6 K using a mass-selected ion beam. Both indene and acyclic precursors were used in an ion source to produce the $C_7H_3^+$ cations which were codeposited with excess of neon to produce the matrix. The electronic absorption spectra were measured by the sensitive waveguide technique sampling around 10^{16} cm^{-3} species. Some of the cations show well-resolved fluorescence. Some neutral C_7H_3 isomers are also detected in absorption produced in the matrix by photo-bleaching of the cations. The charge of the mass-selected species is experimentally established using presence of electron scavengers, release of electrons, changing the kinetic energy during deposition and precursor dependence, whereas the structure of the isomers is inferred by comparison of the energies of the transitions with CASPT2 calculations. The assignment is supported by comparison of the vibrational frequencies inferred from the spectra and theory. The first time identification of the electronic transitions of these structurally interesting isomers provides their means for their *in situ* monitoring in hydrocarbon combustion processes and formation of aromatics therein.